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Single adatom adsorption on metal surfaces by first principles: effects of symmetry gap and surface states on the adatom electronic properties M.I. TRIONI, CNISM and CNR-INFM, UdR Milano Bicocca, Milano, Italy, S. ACHILLI, Dept. Material Science, Univ. Milano-Bicocca, Milano, Italy, E.V. CHULKOV, DIPC and Dept. Material Science (UPV/EHU) and CFM (CSIC-UPV/EHU), San Sebastiàn, Basque Country, Spain — The adsorption of a single atom on an extended substrate is a fundamental step in processes occurring at surfaces. But its theoretical description is still extremely difficult. After the "adatom on jellium" approach by Lang and Williams, only very few methods have been developed in order to treat a single adatom on a more realistic substrate than jellium. In this paper we present a new theoretical approach, within the density functional theory framework, which is able to take into account i) the semi-infinite nature of the substrate, ii) the presence of gap in the surface projected bulk bands, and iii) the existence of surface states. These ingredients are basic for a suitably realistic description of adsorption. We will show the effects of the symmetry gap on the line width of the adsorbate resonances for alkali (Li-Cs), Ba, and magnetic $3d$ adatoms (Ti-Co) on noble metals.

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